

Phenacetin

62-44-2 | DTXSID1021116

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3.76

Global applicability domain: Inside

Local applicability domain index: 5.04e-01

Confidence level: 7.21e-01

Nearest Neighbors from the Training Set

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Bromacil

Measured: 3.24

Predicted: 2.87

Image not found

2-Isopropyl-6-methyl-4-pyrimidone

Measured: 1.82

Predicted: 2.23

Image not found

Molinate

Measured: 25.7

Predicted: 14.8

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Paraldehyde

Measured: 3.02

Predicted: 2.77

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4-Isobutylmorpholine

Measured: 1.78

Predicted: 2.69